Computer Method Gives Alloy Models

Method uses x-ray data, identifies small ordered groups in atomic structure

A digital computer, some rather obscure x-ray diffraction data, a simple idea, and some sophisticated computer programing were combined by the scientists at Northwestern University who developed the newly revealed method for determining the detailed atomic structure of binary alloys (C&EN, Feb. 22, page 35). The method gives the first accurate three-dimensional models of the arrangement of atoms within alloys.

These models identify small, ordered groups of atoms in the generally random matrix of alloys. Knowledge of these groups is vital to materials scientists as these structures help to determine an alloy's properties.

Dr. Jerome B. Cohen of Northwestern's department of materials science, who has been in charge of developing the technique, says that it is based on an idea that is "so simple that it is almost naive." It is a mathematical method based on data measured by x-ray diffraction. Unlike previous attempts to gain a three-dimensional view of alloy structure, the technique does not depend on complicated assumptions about the energy of atoms within an alloy.

Explains. Graduate student Pierre Gehlen is largely responsible for the method. He explains that the data measured by the x-ray studies consist of parameters that give some indications of the over-all (long-range) and local (short-range) arrangements of atoms in a binary alloy. These parameters are programed into a computer that uses them to identify each atom in a mathematically defined matrix. Mr. Gehlen used the parameters from some copper-gold and copper-aluminum alloys in developing the method.

The long-range parameter (S) of an alloy is a direct measure of the fraction of a given atom type that is in a given location on a lattice. In a completely ordered system, such as a crystal of sodium chloride, $S = 1$ as each type of atom is in an assigned sublattice. With a completely random system, $S = 0$. When there is some, but not total, order—as with most alloys—S lies between 1 and 0.

Guides. The short-range order parameters are guides to the tendency for atoms to group in orderly shells around any one atom. These parameters can be measured for the first six shells.

Dr. Lyle Schwartz, also of Northwestern's materials science department, who disclosed Dr. Cohen's and Mr. Gehlen's work at the Chicago meeting of the American Institute of Mining, Metallurgical, and Petroleum Engineers, explains that all these parameters give only averages of particular atomic arrangements. They have been of limited use in the study of alloys; they tell nothing about the arrangements around specific atoms and give no indication of any irregularities that there may be in an alloy's atomic lattice.

To program these parameters into the computer, the Northwestern group starts by defining a matrix of from 4000 to 16,000 atoms—16,000 being the maximum number that the school's IBM 709 can handle conveniently. Using an AB alloy as an example, the equal numbers of A and B atoms are arranged randomly or in some arbitrary, ordered way.

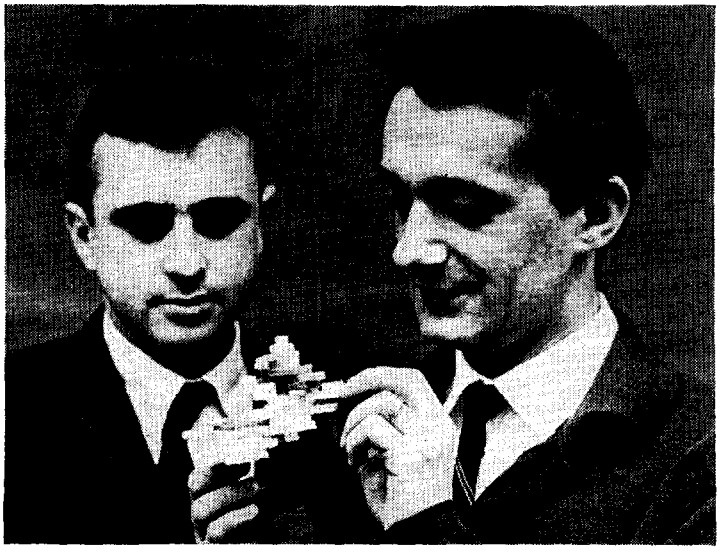
The "ground rules" are then built into the program in the form of the long- and short-range order parameters. These give some guide as to where the A and B atoms should be. The computer then randomly switches atoms from place to place within the matrix until the arrangement is in the best possible agreement with the parameters. During this switching process, a switch is made only if it helps to bring the total arrangement closer to meeting the parameters.

The idea may be simple, but the programing is not. It took two years to perfect, Dr. Cohen says. One of the difficulties is that the computer sometimes needs help, especially toward the end of a run. As the atomic arrangement nears its final form, it becomes difficult for the computer to detect the few atoms that are still out place. At this stage the compu slows down and literally makes o noises to warn the operator of problem. When this happens, m instructions can be fed to the co puter to help it identify the aton that still need moving.

Final. The computer prints o the final result in a series of cha showing two-dimensional slices of t model. These can be stacked at one another to give the three-dime sional model.

The method finds ordered local gions in each of the alloys studie These vary from alloy to alloy. The also vary in any one alloy with temperature. Some of these regions are two-, others are three-dimensional.

The structural models created by the computer check out mathematically. The models were generated using the first one, two, or three of the six available short-range order parameters—the higher-order parameters were not used. But when these higher-order parameters are calculated from the models, they agree well with the observed values from the x-ray studies of the actual alloys.



MODEL. Dr. J. B. Cohen (left) and Pierre Gehlen examine a model of the atomic structure of a copper-gold alloy, assembled from information obtained by their new technique